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Strain-induced tuning of surface energy, electron conductivity, and reduction drive in spinel $LiMn_2O_4$ cathodes[1] IVAN SCIVETT, GILBERTO TEOBALDI, University of Liverpool — $LiMn_2O_4$ (LMO) implementation in rechargeable Li-ion batteries (LIBs) for stationary storage is hampered by the limited lifetime of the material and its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO are related to the surface orientation and reduction drive. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can induce insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], use of strained LMO coating as SEI-formation agent is put forward towards engineering of longer lived SEI on LMO substrates.

1. JCPC 2012, 116, 9852-9861
2. J. Am. Chem. Soc. 2010, 132, 15268-15276
3. J. Phys. Chem. C 2015, 119, 21358-21368
4. ACS Nano 2012, 6, 5531

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